Proc. 9th Int. Conf. Ternary and Multinary Compounds, Yokohama, 1993

Invited

Predictions of New Semiconductor of Transition Metal Structures and Their Properties

Alex ZUNGER

National Renewable Energy Laboratory, Golden, Colorado 80401, USA

(Received September 11, 1993)

I describe how one can use the "Cluster Expansion Method" to predict systematically what are the thermodynamically stable crystal structures on a given lattice type. The method is used to illustrate how both intermetallic compounds can be identified, including

I will discuss here the prospects of the recently developed "cluster expansion methods"[6] which allow one to (i) perform a systematic ground state search among 10^5 atomic configurations and, (ii) obtain the temperature-composition phase diagram in a *first-principles manner*, system.[13] For example, information about the values of the J's may be extracted from experimental critical temperatures.[13] This approach is the simplest, but it provides little new information about the properties of the alloy.

The second approach is to determine the J's by treating

metries established clearly from experiment[24] are also

layer $(AC)_1/(BC)_1$ superlattices in the (111) orientation[32]

ted from the basis set used to extract J_F some of the struc-

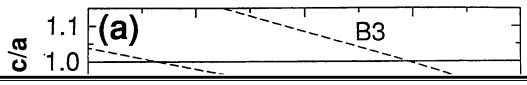
never perfect; it can however, be maximized in certain

grown on GaAs[42] (rather than the alloy). There are now experimental confirmations of this idea.[43] (ii) Use of strain to convert the *indirect* gap Si_nGe_n SL grown on Si

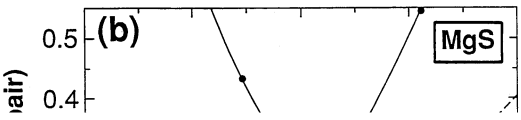
The terms in brackets are the nearest-neighbor terms of eq. (3). All odd terms were omitted, assuming that the Hamiltonian is invariant under the A↔B interchange.

Using the LAPW method we have calculated the

[Fig. 6(b)]. The maximum equilibrium solubility of ZnSe in $CuInSe_2$ with the chalcopyrite structure is 22% (at



order temperature of $CuInSe_2$. Our results hence show that, contrary to the other known heterostructural ternary alloy $(GaAs)_{1-x}Ge_{2x}$, characterized by vanishing solid



2) D. M. Wood and A. Zunger: Phys. Rev B **34** (1986) 4105.
3) A. E. Carlson, D. M. Wood and A. Zunger: Phys. Rev. B **32**
24) P. M. Hansen: *Constitution of Binary Alloys* (McGraw-Hill, New York, 1958).